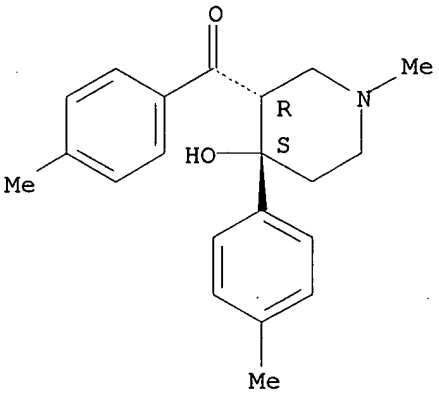
L2 1 S WO2001022964/PN
L3 ANALYZE L2 1 RN : 35 TERMS

FILE 'REGISTRY' ENTERED AT 13:08:27 ON 10 SEP 2003
L4 35 S L3

=> d scan

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidinyl](4-methylphenyl)-, rel-(-)- (9CI)
MF C21 H25 N O2

Rotation (-). Absolute stereochemistry unknown.

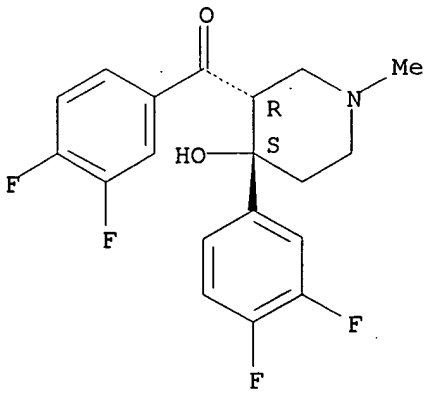


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):34

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (3,4-difluorophenyl)[(3R,4S)-4-(3,4-difluorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI)
MF C19 H17 F4 N O2

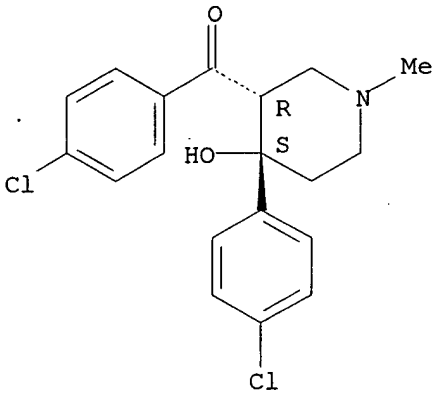
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (4-chlorophenyl)[(3R,4S)-4-(4-chlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI)
MF C19 H19 Cl2 N O2

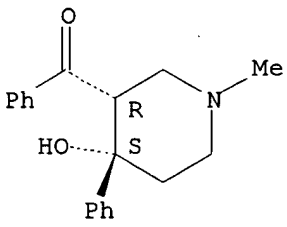
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-phenyl-3-piperidinyl]phenyl-, rel-(-)- (9CI)
MF C19 H21 N O2

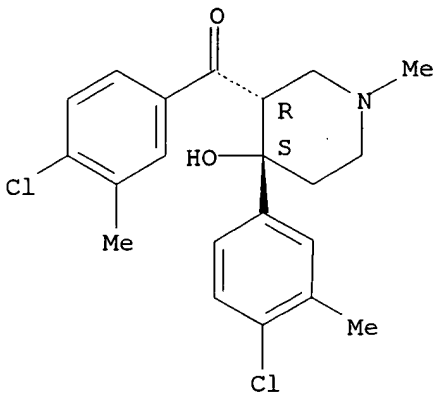
Rotation (-). Absolute stereochemistry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (4-chloro-3-methylphenyl)[(3R,4S)-4-(4-chloro-3-methylphenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, hydrochloride, rel- (9CI)
MF C21 H23 Cl2 N O2 . Cl H

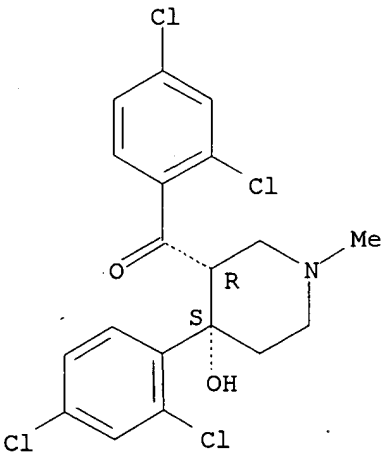
Relative stereochemistry.



● HCl

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (2,4-dichlorophenyl)[(3R,4S)-4-(2,4-dichlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI)
MF C19 H17 Cl4 N O2

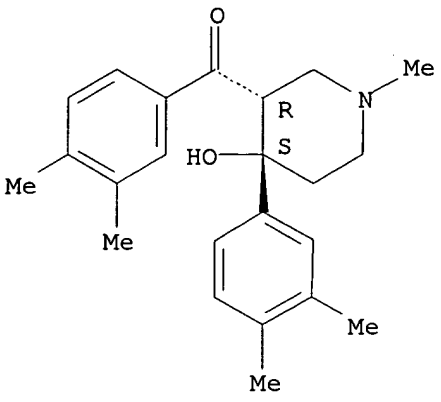
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (3,4-dimethylphenyl)[(3R,4S)-4-(3,4-dimethylphenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, hydrochloride, rel-(-)- (9CI)
MF C23 H29 N O2 . Cl H

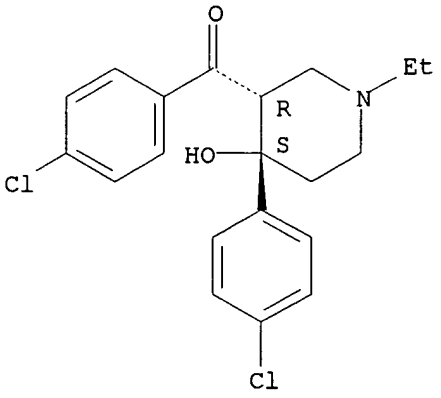
Rotation (-). Absolute stereochemistry unknown.



● HCl

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (4-chlorophenyl)[(3R,4S)-4-(4-chlorophenyl)-1-ethyl-4-hydroxy-3-piperidinyl]-, rel- (9CI)
MF C20 H21 Cl2 N O2
CI COM

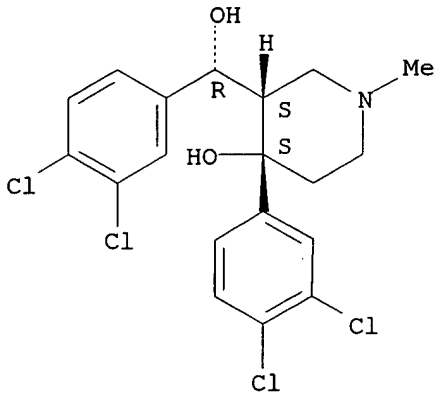
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 3-Piperidinemethanol, .alpha.,4-bis(3,4-dichlorophenyl)-4-hydroxy-1-methyl-, (.alpha.R,3S,4S)-rel- (9CI)
MF C19 H19 Cl4 N O2

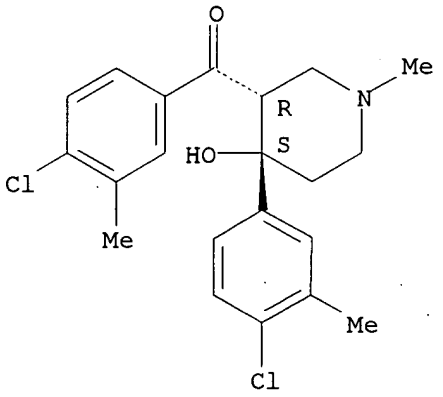
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (4-chloro-3-methylphenyl)[(3R,4S)-4-(4-chloro-3-methylphenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, hydrochloride, rel-(-)- (9CI)
MF C21 H23 Cl2 N O2 . Cl H

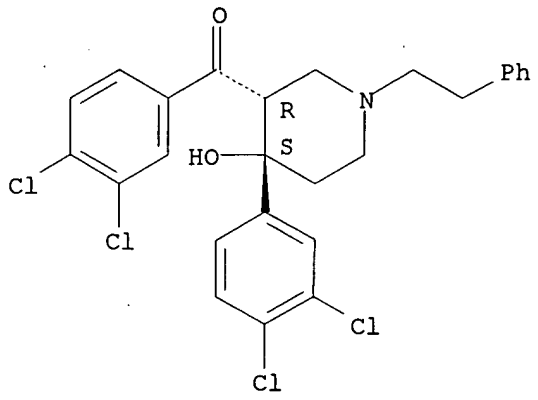
Rotation (-). Absolute stereochemistry unknown.



● HCl

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (3,4-dichlorophenyl)[(3R,4S)-4-(3,4-dichlorophenyl)-4-hydroxy-1-(2-phenylethyl)-3-piperidinyl]-, hydrochloride, rel- (9CI)
MF C26 H23 Cl4 N O2 . Cl H

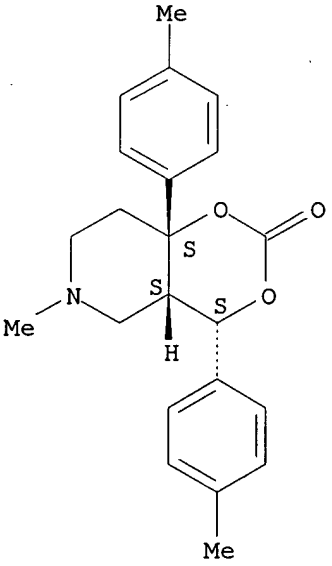
Relative stereochemistry.



● HCl

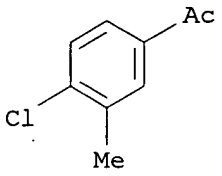
L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 4H-1,3-Dioxino[5,4-c]pyridin-2-one, hexahydro-6-methyl-4,8a-bis(4-methylphenyl)-, (4R,4aR,8aR)-rel- (9CI)
MF C22 H25 N O3

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

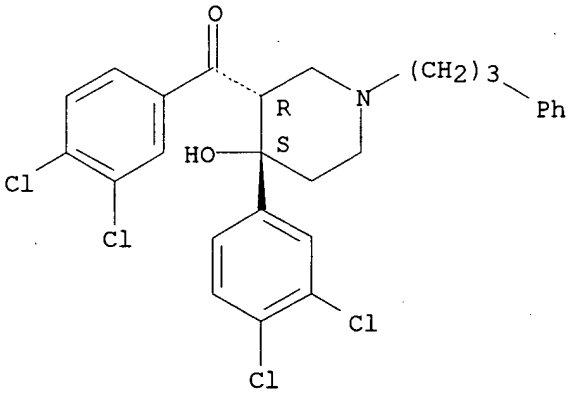
L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Ethanone, 1-(4-chloro-3-methylphenyl)- (9CI)
MF C9 H9 Cl O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (3,4-dichlorophenyl)[(3R,4S)-4-(3,4-dichlorophenyl)-4-hydroxy-1-(3-phenylpropyl)-3-piperidinyl]-, rel- (9CI)
MF C27 H25 Cl4 N O2

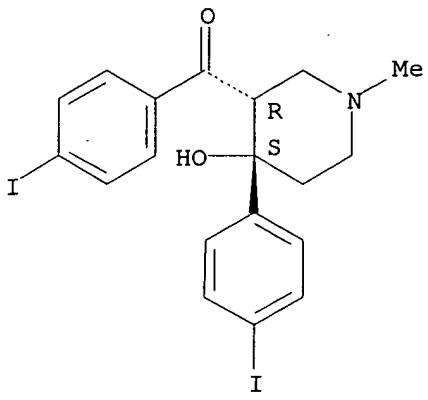
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, [(3R,4S)-4-hydroxy-4-(4-iodophenyl)-1-methyl-3-piperidinyl](4-iodophenyl)-, rel- (9CI)
MF C19 H19 I2 N O2

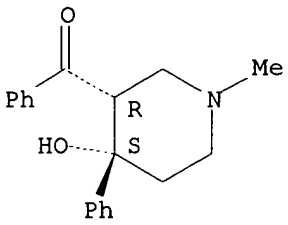
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-phenyl-3-piperidinyl]phenyl-, rel- (9CI)
MF C19 H21 N O2
CI COM

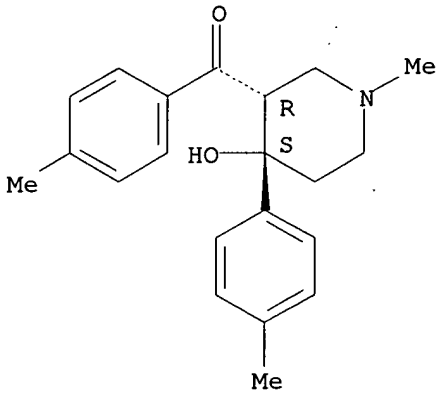
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidinyl](4-methylphenyl)-, rel-(+)- (9CI)
MF C21 H25 N O2

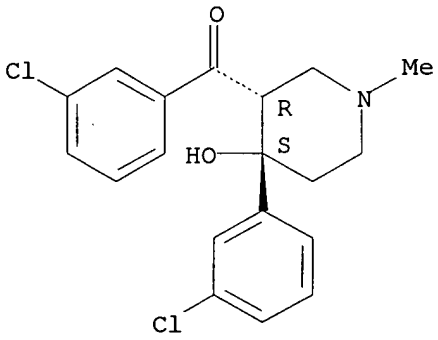
Rotation (+). Absolute stereochemistry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (3-chlorophenyl)[(3R,4S)-4-(3-chlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI)
MF C19 H19 Cl2 N O2

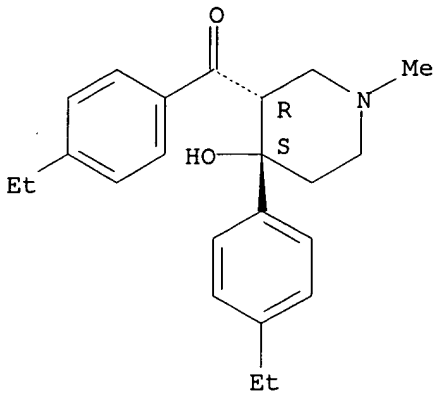
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (4-ethylphenyl)[(3R,4S)-4-(4-ethylphenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI)
MF C23 H29 N O2

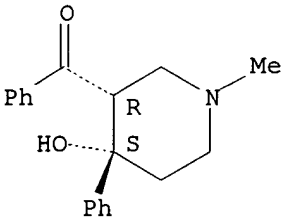
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-phenyl-3-piperidinyl]phenyl-, rel-(+)- (9CI)
MF C19 H21 N O2

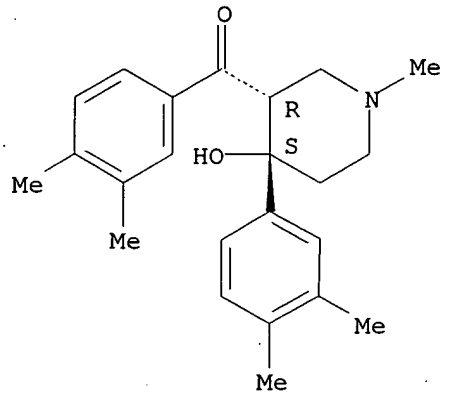
Rotation (+). Absolute stereochemistry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (3,4-dimethylphenyl)[(3R,4S)-4-(3,4-dimethylphenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, hydrochloride, rel- (9CI)
MF C23 H29 N O2 . Cl H

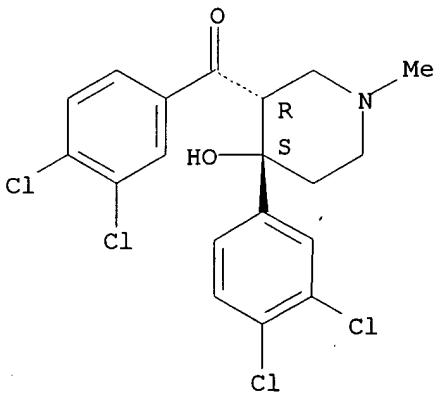
Relative stereochemistry.



● HCl

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (3,4-dichlorophenyl)[(3R,4S)-4-(3,4-dichlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI)
MF C19 H17 Cl4 N O2

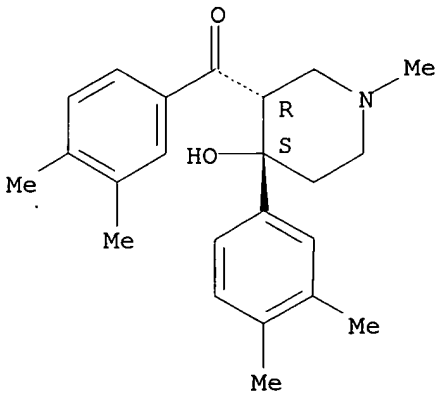
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (3,4-dimethylphenyl)[(3R,4S)-4-(3,4-dimethylphenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, hydrochloride, rel-(+)- (9CI)
MF C23 H29 N O2 . Cl H

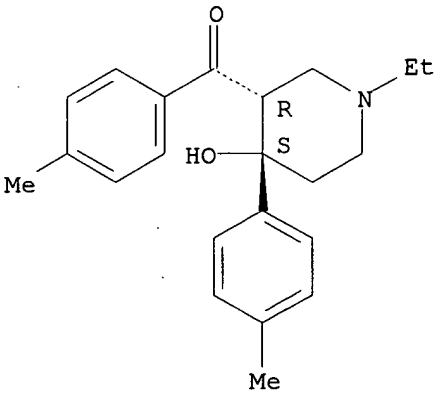
Rotation (+). Absolute stereochemistry unknown.



● HCl

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, [(3R,4S)-1-ethyl-4-hydroxy-4-(4-methylphenyl)-3-piperidinyl](4-methylphenyl)-, rel- (9CI)
MF C22 H27 N O2
CI COM

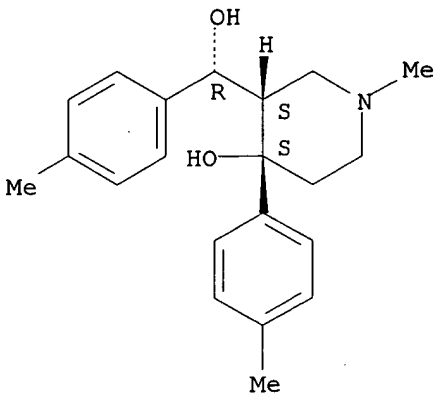
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 3-Piperidinemethanol, 4-hydroxy-1-methyl-.alpha.,4-bis(4-methylphenyl)-, (.alpha.R,3S,4S)-rel- (9CI)
MF C21 H27 N O2

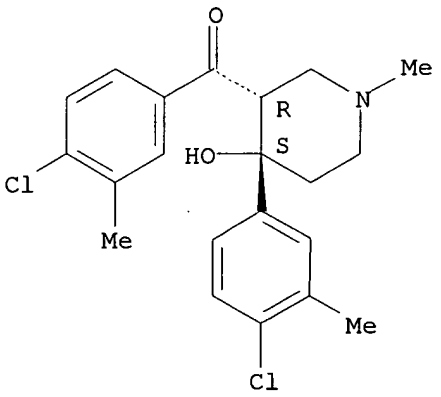
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (4-chloro-3-methylphenyl)[(3R,4S)-4-(4-chloro-3-methylphenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, hydrochloride, rel-(+)- (9CI)
MF C21 H23 Cl2 N O2 . Cl H

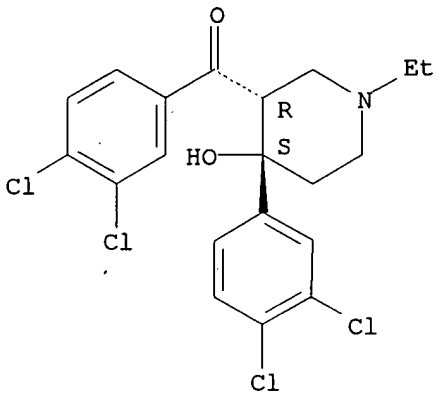
Rotation (+). Absolute stereochemistry unknown.



● HCl

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (3,4-dichlorophenyl)[(3R,4S)-4-(3,4-dichlorophenyl)-1-ethyl-4-hydroxy-3-piperidinyl]-, rel- (9CI)
MF C20 H19 Cl4 N O2
CI COM

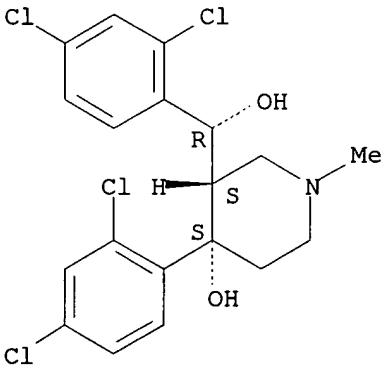
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 3-Piperidinemethanol, .alpha.,4-bis(2,4-dichlorophenyl)-4-hydroxy-1-methyl-, (.alpha.R,3S,4S)-rel- (9CI)
MF C19 H19 Cl4 N O2

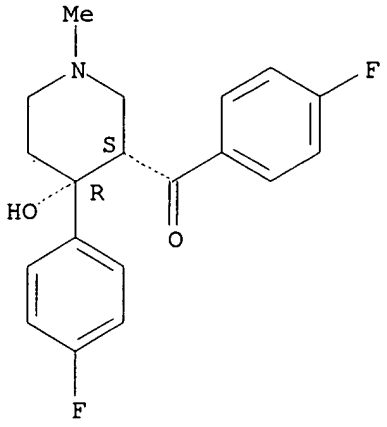
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (4-fluorophenyl)[(3R,4S)-4-(4-fluorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI)
MF C19 H19 F2 N O2

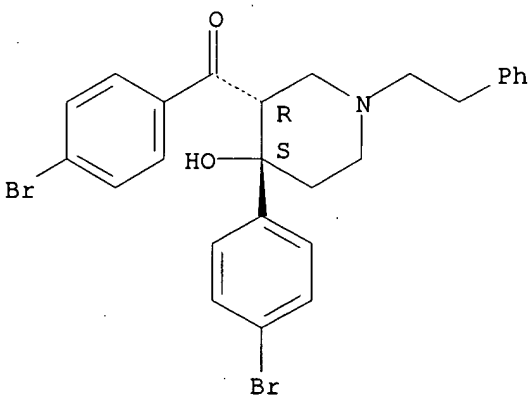
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (4-bromophenyl)[(3R,4S)-4-(4-bromophenyl)-4-hydroxy-1-(2-phenylethyl)-3-piperidinyl]-, rel- (9CI)
MF C26 H25 Br2 N O2

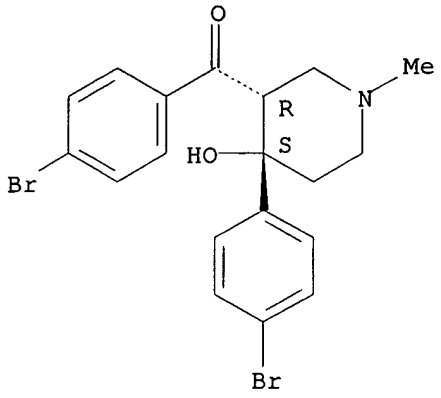
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

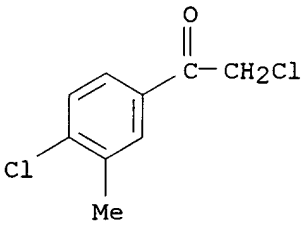
L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (4-bromophenyl)[(3R,4S)-4-(4-bromophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI)
MF C19 H19 Br2 N O2
CI COM

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

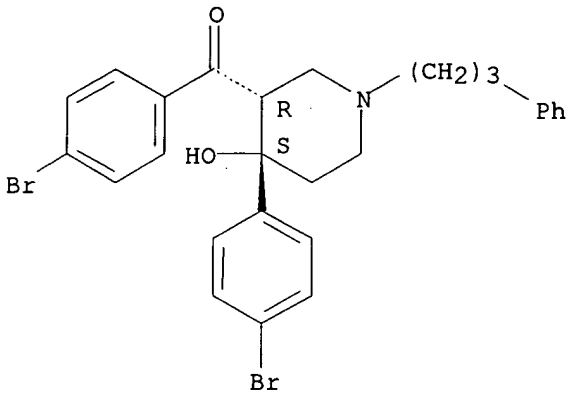
L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Ethanone, 2-chloro-1-(4-chloro-3-methylphenyl)- (9CI)
MF C9 H8 Cl2 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (4-bromophenyl)[(3R,4S)-4-(4-bromophenyl)-4-hydroxy-1-(3-phenylpropyl)-3-piperidinyl]-, rel- (9CI)
MF C27 H27 Br2 N O2

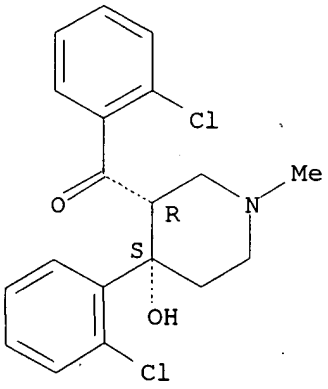
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, (2-chlorophenyl)[(3R,4S)-4-(2-chlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI)
MF C19 H19 Cl2 N O2

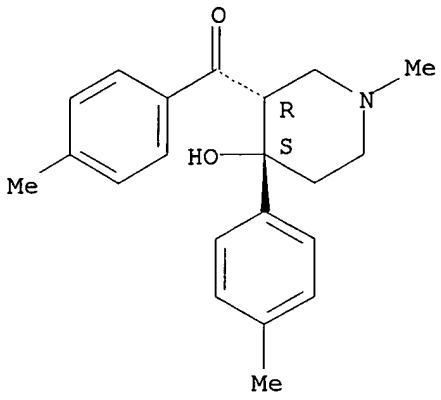
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 35 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidinyl](4-methylphenyl)-, rel- (9CI)
MF C21 H25 N O2

Relative stereochemistry.

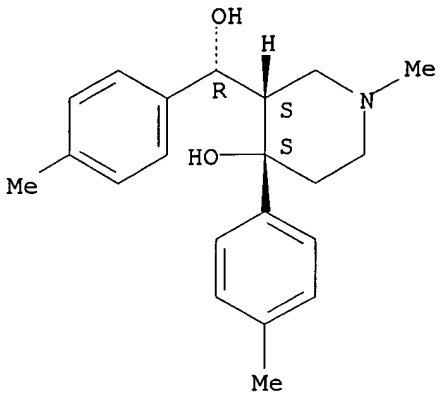


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

AN 2000:44073 CAPLUS
DN 132:216547
TI Discovery of a novel dopamine transporter inhibitor, 4-Hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidyl 4-methylphenyl ketone, as a potential cocaine antagonist through 3D-database pharmacophore searching. Molecular modeling, structure-activity relationships, and behavioral pharmacological studies
AU Wang, Shaomeng; Sakamuri, Sukumar; Enyedy, Istvan J.; Kozikowski, Alan P.; Deschaux, Olivier; Bandyopadhyay, Bidhan C.; Tella, Srihari R.; Zaman, Wahiduz A.; Johnson, Kenneth M.
CS Drug Discovery Program Georgetown Institute for Cognitive and Computational Science, Georgetown University Medical Center, Washington, DC, 20007, USA
SO Journal of Medicinal Chemistry (2000), 43(3), 351-360
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB A novel, fairly potent dopamine transporter (DAT) inhibitor, 4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidyl 4-methylphenyl ketone (3, Ki values of 492 and 360 nM in binding affinity and inhibition of dopamine reuptake, resp.), with significant functional antagonism against cocaine and a different in vitro pharmacol. profile from cocaine at the three transporter sites (dopamine, serotonin, and norepinephrine) was discovered through 3D-database pharmacophore searching. Through structure-activity relationships and mol. modeling studies, we found that hydrophobicity and conformational preference are two addnl. important parameters that det. affinity at the DAT site. Chem. modifications of the lead compd. (3) led to a high affinity analog (6, Ki values of 11 and 55 nM in binding affinity and inhibition of dopamine reuptake, resp.). In behavioral pharmacol. testing, 6 mimics partially the effect of cocaine in increasing locomotor activity in mice but lacks cocaine-like discriminative stimulus effect in rats. Taken together, these data suggest that 6 represents a promising lead for further evaluations as potential therapy for the treatment of cocaine abuse.
IT **260969-80-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(hydroxymethylmethylphenylpiperidyl methylphenyl ketone, novel dopamine transporter inhibitor, as a potential cocaine antagonist)
RN 260969-80-0 CAPLUS
CN 3-Piperidinemethanol, 4-hydroxy-1-methyl-.alpha.,4-bis(4-methylphenyl)-, (.alpha.R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

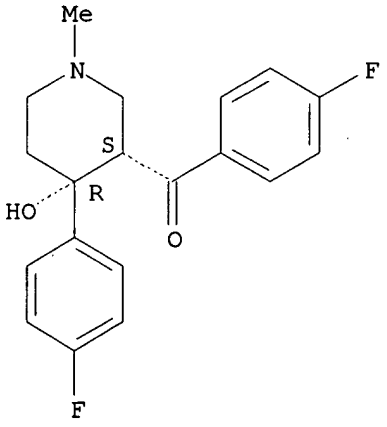


IT **31088-27-4P 224948-86-1P 224948-87-2P 260969-78-6P 260969-79-7P 260969-81-1P 260969-82-2P 260969-83-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(hydroxymethylmethylphenylpiperidyl methylphenyl ketone, novel dopamine transporter inhibitor, as a potential cocaine antagonist)

RN 31088-27-4 CAPLUS

CN Methanone, (4-fluorophenyl)[(3R,4S)-4-(4-fluorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

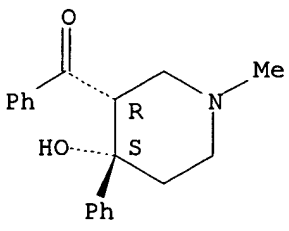
Relative stereochemistry.

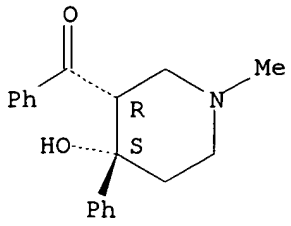


RN 224948-86-1 CAPLUS

CN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-phenyl-3-piperidinyl]phenyl-, rel- (9CI) (CA INDEX NAME)

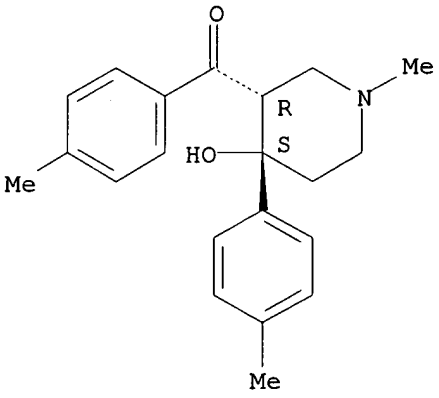
Relative stereochemistry.





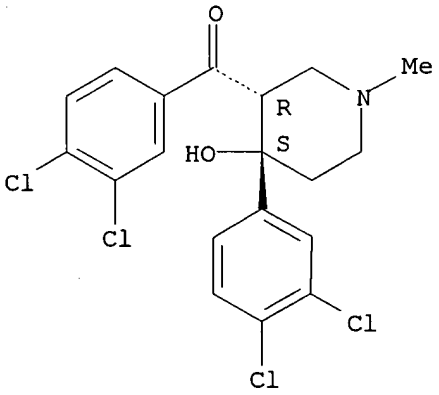
RN 224948-87-2 CAPLUS
CN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidinyl](4-methylphenyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



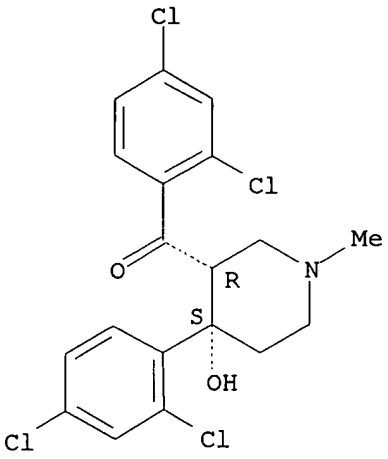
RN 260969-78-6 CAPLUS
CN Methanone, (3,4-dichlorophenyl)[(3R,4S)-4-(3,4-dichlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



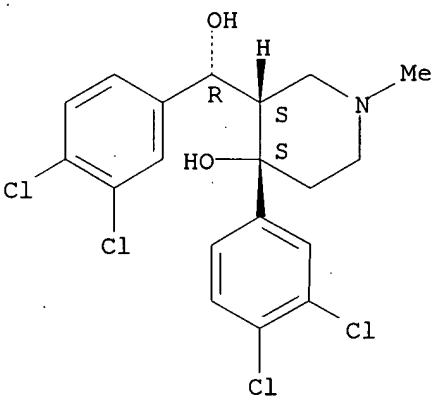
RN 260969-79-7 CAPLUS
CN Methanone, (2,4-dichlorophenyl)[(3R,4S)-4-(2,4-dichlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



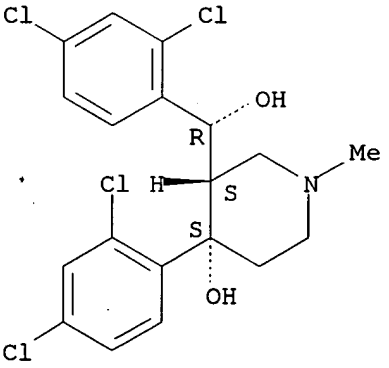
RN 260969-81-1 CAPLUS
CN 3-Piperidinemethanol, .alpha.,4-bis(3,4-dichlorophenyl)-4-hydroxy-1-methyl-, (.alpha.R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 260969-82-2 CAPLUS
CN 3-Piperidinemethanol, .alpha.,4-bis(2,4-dichlorophenyl)-4-hydroxy-1-methyl-, (.alpha.R,3S,4S)-rel- (9CI) (CA INDEX NAME)

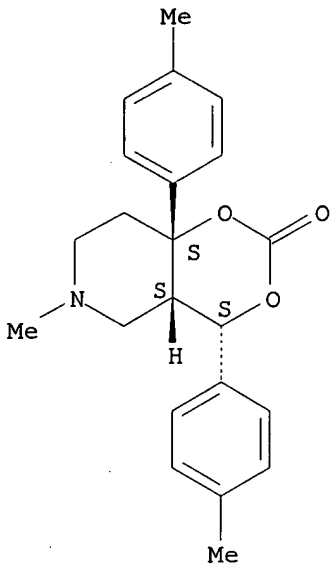
Relative stereochemistry.



RN 260969-83-3 CAPLUS

CN 4H-1,3-Dioxino[5,4-c]pyridin-2-one, hexahydro-6-methyl-4,8a-bis(4-methylphenyl)-, (4R,4aR,8aR)-rel- (9CI) (CA INDEX NAME)

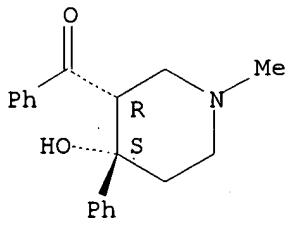
Relative stereochemistry.



RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

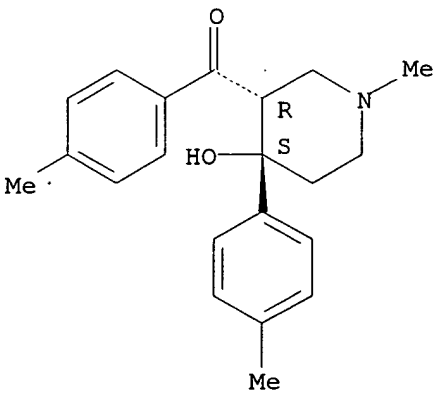
AN 1999:208020 CAPLUS
DN 130:351978
TI Phenindamine and its analogs and precursors: NMR evidence of structure and configuration
AU Casy, Alan F.; Hussain, Rohannah B.; Upton, Christopher
CS School of Pharmacy and Pharmacology, University of Bath, Bath, BA2 7AY, UK
SO Magnetic Resonance in Chemistry (1992), 30(7), 621-625
CODEN: MRCHEG; ISSN: 0749-1581
PB John Wiley & Sons Ltd.
DT Journal
LA English
AB The 1H and 13C NMR spectra of analogs of the antihistaminic agent phenindamine and its precursors are interpreted in terms of structure and geometry. Points of interest are the conformations of 4-piperidinol and dihydro-1-pyrindene(diene) intermediates, and the configuration of the hexahydro analog of phenindamine and its corresponding product of equilibration. Results of an antihistamine evaluation test are presented.
IT **224948-86-1 224948-87-2 224948-90-7**
RL: PRP (Properties)
(NMR study of structure and configuration of phenindamine and its analogs and precursors)
RN 224948-86-1 CAPLUS
CN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-phenyl-3-piperidinyl]phenyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 224948-87-2 CAPLUS
CN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidinyl](4-methylphenyl)-, rel- (9CI) (CA INDEX NAME)

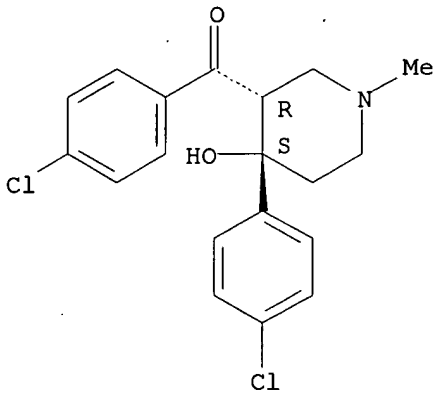
Relative stereochemistry.



RN 224948-90-7 CAPLUS
CN Methanone, (4-chlorophenyl)[(3R,4S)-4-(4-chlorophenyl)-4-hydroxy-1-methyl-

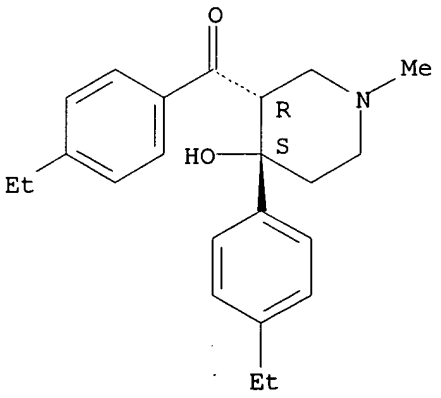
3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **224948-88-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(NMR study of structure and configuration of phenindamine and its analogs and precursors)
RN 224948-88-3 CAPLUS
CN Methanone, (4-ethylphenyl)[(3R,4S)-4-(4-ethylphenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

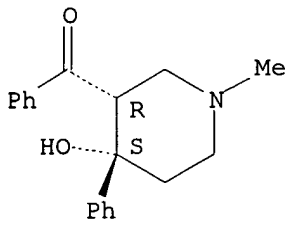
Relative stereochemistry.



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

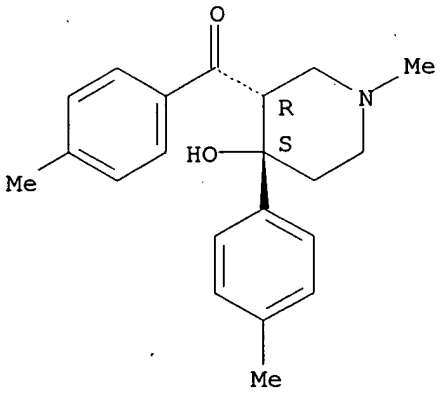
AN 2000:419973 CAPLUS
DN 133:171745
TI Conformationally-restricted ligands for the histamine H1 receptor
AU Upton, Christopher; Osborne, Richard H.; Jaffar, Mohammad
CS Department of Pharmacy and Pharmacology, University of Bath, Bath, BA2 7AY, UK
SO Bioorganic & Medicinal Chemistry Letters (2000), 10(11), 1277-1279
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
AB Potent H1-antagonistic activity in a series of novel indeno[2,1-c]pyridines and their 4-arylpiperidinol precursors is reported; one compd. shows an in vitro activity four times that of the std. mepyramine that it was screened against. Their failure to translate this protection to in vivo tests is discussed.
IT **224948-86-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(conformationally-restricted ligands for histamine H1 receptor)
RN 224948-86-1 CAPLUS
CN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-phenyl-3-piperidinyl]phenyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



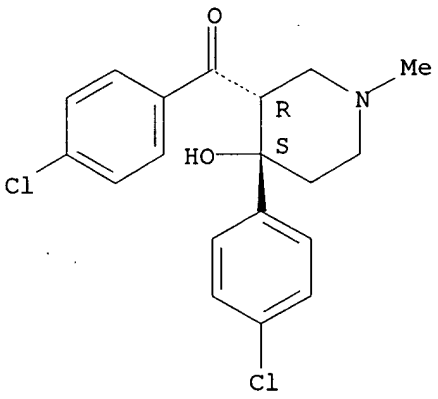
IT **224948-87-2 224948-90-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(conformationally-restricted ligands for histamine H1 receptor)
RN 224948-87-2 CAPLUS
CN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidinyl](4-methylphenyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 224948-90-7 CAPLUS
CN Methanone, (4-chlorophenyl)[(3R,4S)-4-(4-chlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

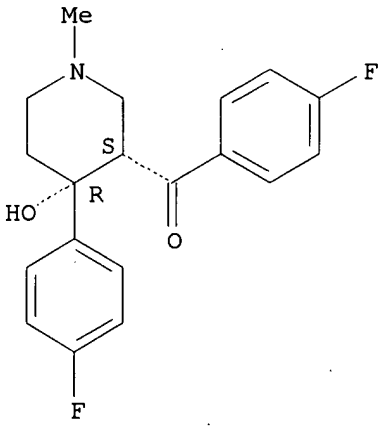
Relative stereochemistry.



RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

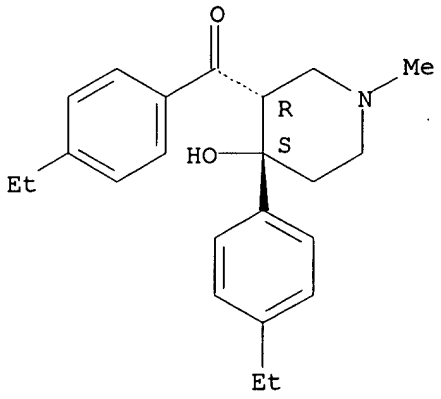
AN 1971:68906 CAPLUS
DN 74:68906
TI Stereochemistry of N-methyl-3-(p-fluoro-benzoyl)-4-hydroxy-4-(p-fluorophenyl)piperidine
AU Draper, Marshall D.; Petracek, Francis J.; Klohs, Murle W.; Parker, Richard Ghrist; Roberts, John D.
CS Chem. Res. Dep., Riker Lab., Inc., Northridge, CA, USA
SO Tetrahedron Letters (1970), (51), 4481-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
AB NMR showed that the title compd. (I) had the piperidine ring in the chair conformation and the p-FC6H4 and p-FC6H4CO groups in the trans-conformation. I crystd. in the monoclinic space group P21/c, with a 17.763, b 7.198, c 16.097 .ANG., and .beta. 113.11.degree..
IT **31088-27-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 31088-27-4 CAPLUS
CN Methanone, (4-fluorophenyl)[(3R,4S)-4-(4-fluorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



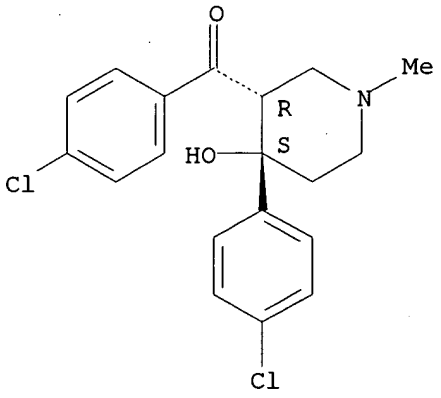
AN 2001:466983 CAPLUS
DN 135:339052
TI Molecular Modeling, Structure-Activity Relationships and Functional Antagonism Studies of 4-Hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidyl 4-Methylphenyl Ketones as a Novel Class of Dopamine Transporter Inhibitors
AU Wang, S.; Sakamuri, S.; Enyedy, I. J.; Kozikowski, A. P.; Zaman, W. A.; Johnson, K. M.
CS Departments of Oncology and Neuroscience, Georgetown University Medical Center, Washington, DC, 20007, USA
SO Bioorganic & Medicinal Chemistry (2001), 9(7), 1753-1764
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English
AB We previously disclosed the discovery of 4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidyl 4-methylphenyl ketone (3) as a novel class of dopamine transporter (DAT) inhibitors and showed that (.+-.)-3 has a significant functional antagonism against cocaine in vitro. Our previous preliminary structure-activity relationship study led to identification of a more potent DAT inhibitor [(.+-.)-4] but this compd. failed to show any significant functional antagonism. To search for more potent analogs than 3 but still displaying significant functional antagonism, further SARs, mol. modeling studies and in vitro pharmacol. evaluation of this novel class of DAT inhibitors were performed. Sixteen new analogs were synthesized in racemic form and evaluated as DAT inhibitors. It was found that seven new analogs are reasonably potent DAT inhibitors with Ki values of 0.041-0.30 and 0.052-0.16 .mu.M in [3H]mazindol binding and inhibition of dopamine (DA) re-uptake. Chiral isomers of several potent DAT inhibitors were obtained through chiral HPLC sepn. and evaluated as inhibitors at all the three monoamine transporter sites. In general, the (-)-isomer is more active than the (+)-isomer in inhibition of DA re-uptake and all the (-)-isomers are selective inhibitors at the DAT site. Evaluation of cocaine's effect on dopamine uptake in the presence and absence of (+)-3 and (-)-3 showed that (-)-3 is responsible for the functional antagonism obtained with the original lead (.+-.)-3. Out of the new compds. synthesized, analog (.+-.)-20, which is 8- and 3-fold more potent than (.+-.)-3 in binding and inhibition of DA re-uptake, appeared to have improved functional antagonism as compared to (.+-.)-3. 4-Hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidyl 4-methylphenyl ketones as a novel class of dopamine transporter inhibitors that display significant in vitro functional antagonism against cocaine.
IT **224948-88-3P 224948-90-7P 332909-01-0P**
332909-04-3P 332909-07-6P 332909-09-8P
332909-11-2P 332909-17-8P 332909-19-0P
332909-21-4P 332909-25-8P 332909-27-0P
332909-29-2P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(prepn., mol. modeling, structure-activity relationships and functional antagonism studies of 4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidyl 4-methylphenyl ketones as a novel class of dopamine transporter inhibitors)
RN 224948-88-3 CAPLUS
CN Methanone, (4-ethylphenyl)[(3R,4S)-4-(4-ethylphenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



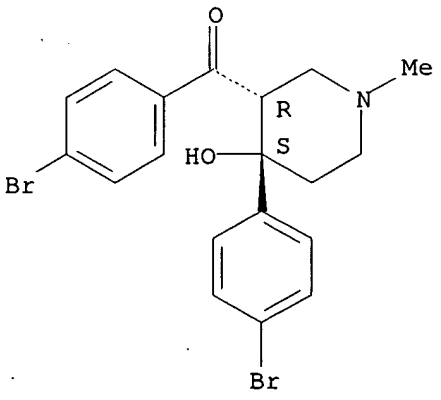
RN 224948-90-7 CAPLUS
CN Methanone, (4-chlorophenyl)[(3R,4S)-4-(4-chlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 332909-01-0 CAPLUS
CN Methanone, (4-bromophenyl)[(3R,4S)-4-(4-bromophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

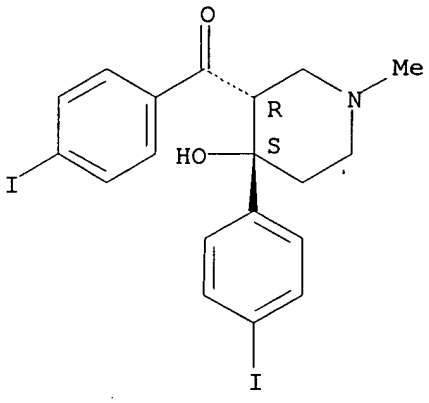
Relative stereochemistry.



RN 332909-04-3 CAPLUS
CN Methanone, [(3R,4S)-4-hydroxy-4-(4-iodophenyl)-1-methyl-3-piperidinyl](4-

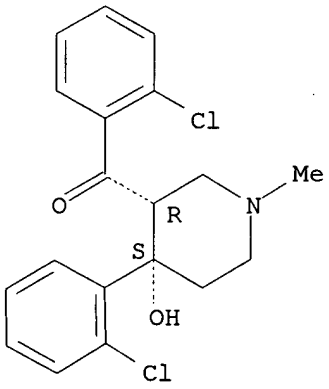
iodophenyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



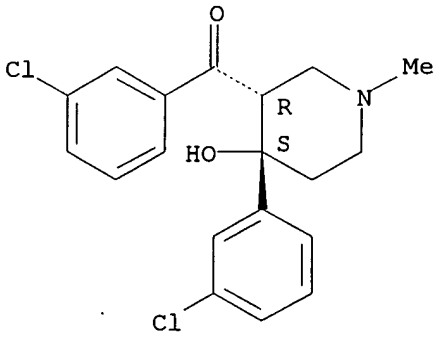
RN 332909-07-6 CAPLUS
CN Methanone, (2-chlorophenyl)[(3R,4S)-4-(2-chlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



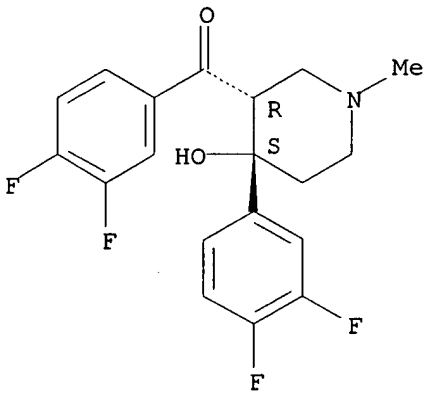
RN 332909-09-8 CAPLUS
CN Methanone, (3-chlorophenyl)[(3R,4S)-4-(3-chlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



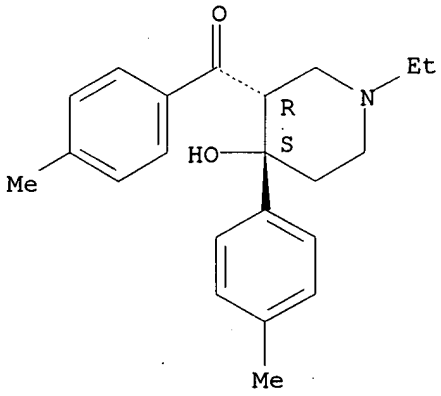
RN 332909-11-2 CAPLUS
CN Methanone, (3,4-difluorophenyl)[(3R,4S)-4-(3,4-difluorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



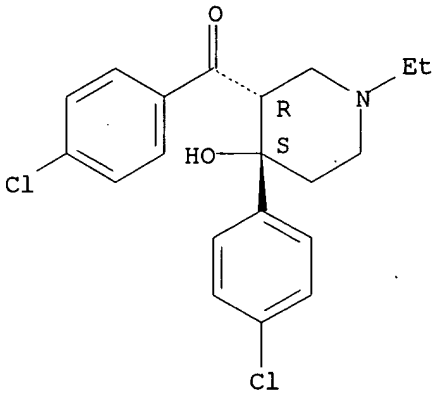
RN 332909-17-8 CAPLUS
CN Methanone, [(3R,4S)-1-ethyl-4-hydroxy-4-(4-methylphenyl)-3-piperidinyl](4-methylphenyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



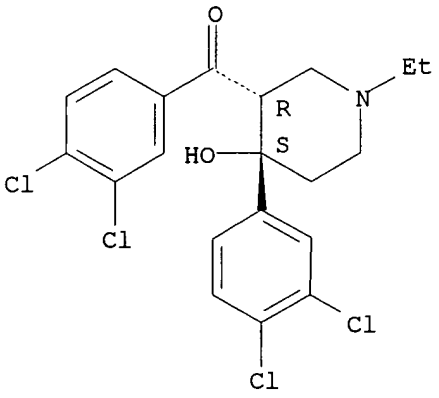
RN 332909-19-0 CAPLUS
CN Methanone, (4-chlorophenyl)[(3R,4S)-4-(4-chlorophenyl)-1-ethyl-4-hydroxy-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



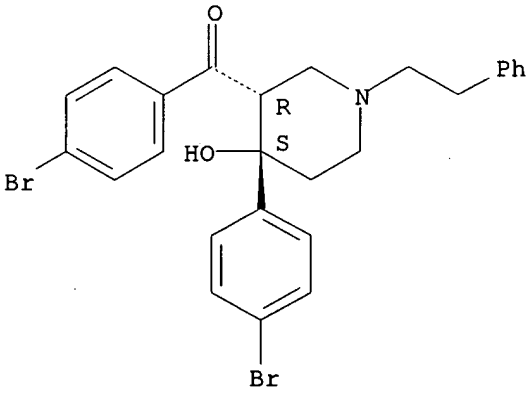
RN 332909-21-4 CAPLUS
CN Methanone, (3,4-dichlorophenyl)[(3R,4S)-4-(3,4-dichlorophenyl)-1-ethyl-4-hydroxy-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 332909-25-8 CAPLUS
CN Methanone, (4-bromophenyl)[(3R,4S)-4-(4-bromophenyl)-4-hydroxy-1-(2-phenylethyl)-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

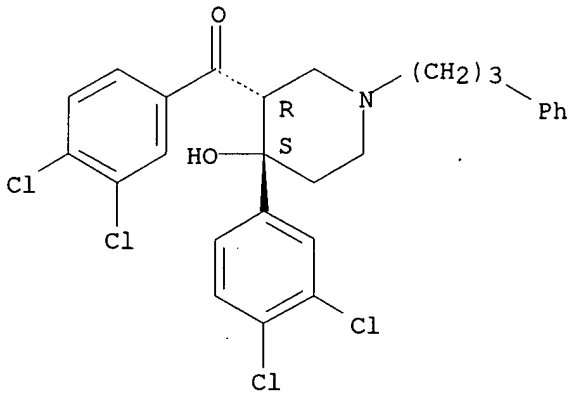
Relative stereochemistry.



RN 332909-27-0 CAPLUS
CN Methanone, (3,4-dichlorophenyl)[(3R,4S)-4-(3,4-dichlorophenyl)-4-hydroxy-1-

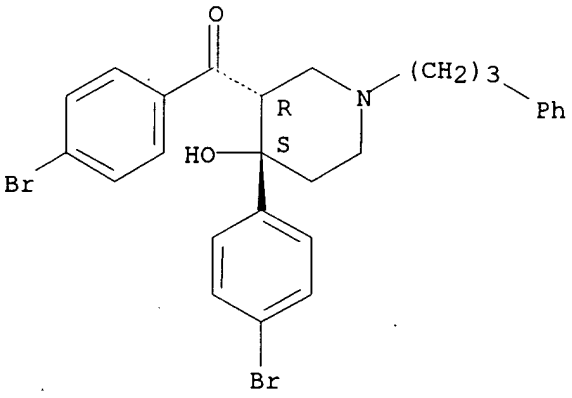
(3-phenylpropyl)-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 332909-29-2 CAPLUS
CN Methanone, (4-bromophenyl)[(3R,4S)-4-(4-bromophenyl)-4-hydroxy-1-(3-phenylpropyl)-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

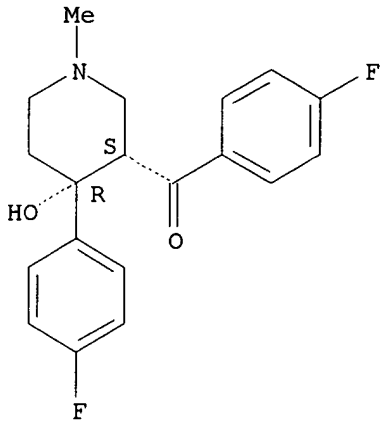
Relative stereochemistry.



IT **31088-27-4 224948-86-1 224948-87-2**
260969-78-6 260969-79-7 260969-80-0
260969-81-1 260969-82-2 260969-83-3
332909-31-6 332909-33-8
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(prepn., mol. modeling, structure-activity relationships and functional antagonism studies of 4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidyl 4-methylphenyl ketones as a novel class of dopamine transporter inhibitors)

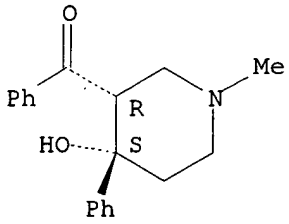
RN 31088-27-4 CAPLUS
CN Methanone, (4-fluorophenyl)[(3R,4S)-4-(4-fluorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



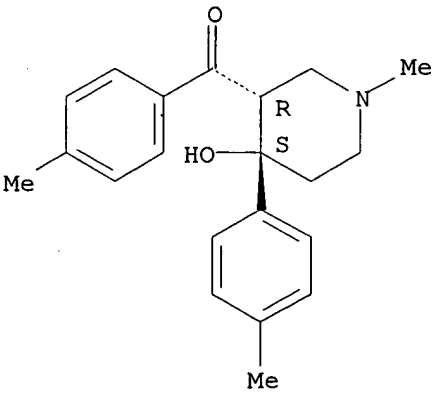
RN 224948-86-1 CAPLUS
CN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-phenyl-3-piperidinyl]phenyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



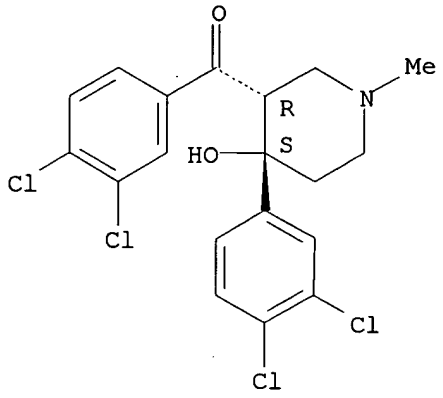
RN 224948-87-2 CAPLUS
CN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidinyl](4-methylphenyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



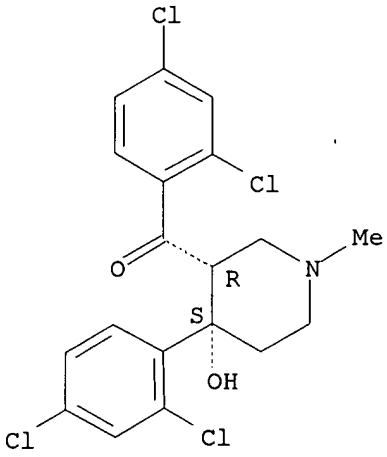
RN 260969-78-6 CAPLUS
CN Methanone, (3,4-dichlorophenyl)[(3R,4S)-4-(3,4-dichlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



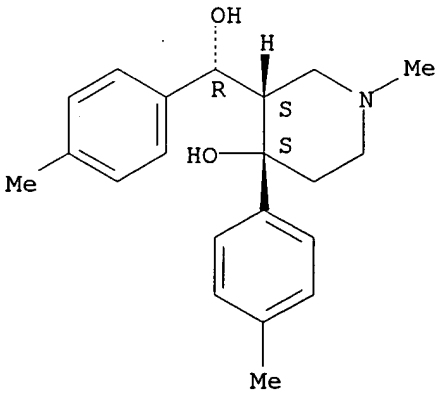
RN 260969-79-7 CAPLUS
CN Methanone, (2,4-dichlorophenyl)[(3R,4S)-4-(2,4-dichlorophenyl)-4-hydroxy-1-methyl-3-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



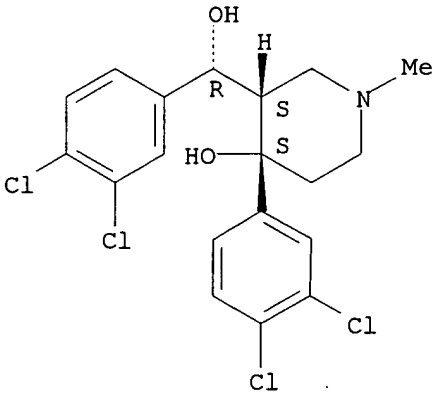
RN 260969-80-0 CAPLUS
CN 3-Piperidinemethanol, 4-hydroxy-1-methyl-.alpha.,4-bis(4-methylphenyl)-, (.alpha.R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



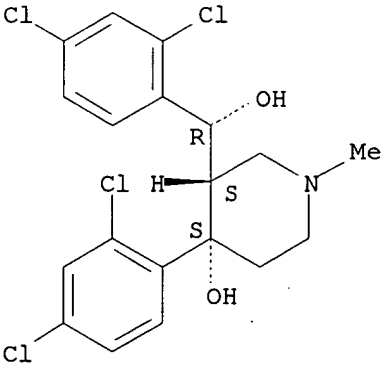
RN 260969-81-1 CAPLUS
CN 3-Piperidinemethanol, .alpha.,4-bis(3,4-dichlorophenyl)-4-hydroxy-1-methyl-, (.alpha.R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



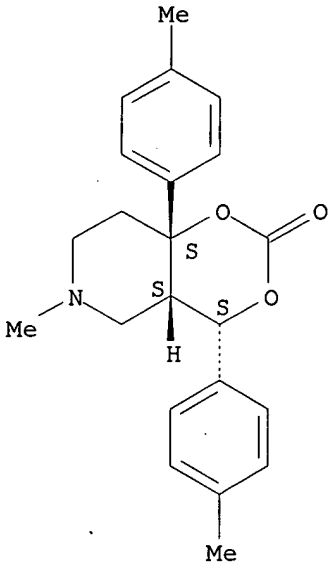
RN 260969-82-2 CAPLUS
CN 3-Piperidinemethanol, .alpha.,4-bis(2,4-dichlorophenyl)-4-hydroxy-1-methyl-, (.alpha.R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



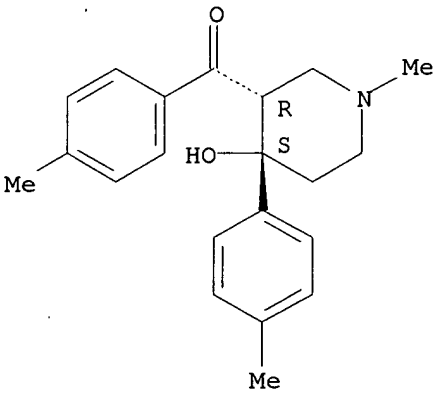
RN 260969-83-3 CAPLUS
CN 4H-1,3-Dioxino[5,4-c]pyridin-2-one, hexahydro-6-methyl-4,8a-bis(4-methylphenyl)-, (4R,4aR,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



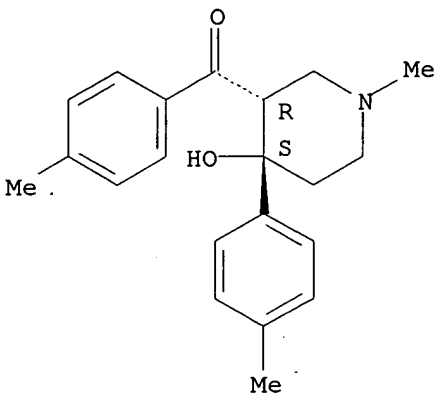
RN 332909-31-6 CAPLUS
CN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidinyl](4-methylphenyl)-, rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



RN 332909-33-8 CAPLUS
CN Methanone, [(3R,4S)-4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidinyl](4-methylphenyl)-, rel-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT